BILLION PARTICLE LINAC SIMULATIONS FOR FUTURE LIGHT SOURCES*

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Abstract

In this paper we report on multi-physics, multi-billion macroparticle simulation of beam transport in a free electron laser (FEL) linac for future light source applications. The simulation includes a self-consistent calculation of 3D space-charge effects, short-range geometry wakefields, longitudinal coherent synchrotron radiation (CSR) wakefields, and detailed modeling of RF acceleration and focusing. We discuss the need for and the challenges associated with such large-scale simulation. Applications to the study of the microbunching instability in an FEL linac are also presented.

INTRODUCTION

The electron beam quality at the entrance to FEL undulators plays a crucial role for the success of next generation X-ray light sources. In order to achieve good performance of X-ray output with reasonable cost, the emittance of the electron beam and the energy spread of the electron beam need to be controlled within the tolerance level subject to a high peak current. However, collective effects such as the microbunching instability driven by space-charge, wakefields, and CSR can pose a particular challenge that leads to irreversible degradation in beam quality. In order to accurately predict the beam properties at the end of linac subject to those collective effects and to optimize the linac design, large-scale self-consistent simulation is needed. As will be shown, the use of on the order of a billion macroparticles or close to real number of electrons per bunch in self-consistent particle tracking helps to correctly simulate the shot noise inside the electron beam that can be amplified by the microbunching instability.

COMPUTATIONAL AND PHYSICAL MODELS

In this study, we have used the IMPACT code [1], a parallel beam dynamics macroparticle tracking code, as our major simulation tool. The IMPACT code is an object-based parallel particle-in-cell code to simulate high intensity, high brightness beam transport in a beam delivery system. It uses a split-operator method to separate the particle advance subject to the given external fields from the particle advance subject to the collective self-consistent space-charge or wakefield forces. The space-charge forces are calculated from the solution of the 3D Poisson equation in the beam frame using a convolution of the charge density with the Green function for open boundary conditions (in most applications). This convolution is calculated numerically on a 3D grid using an integrated Green function method [2] with FFT calculation of a cyclic summation in a doubled computational domain [3]. The space-charge fields are Lorentz transformed back to the laboratory frame to advance particle momentum. The wakefield forces are calculated in the laboratory frame using a convolution of the wake function and the particle density. This convolution is also computed using the FFT based method. The CSR effects inside a chicane are calculated using a one-dimensional longitudinal CSR wake model [4]. As a test of our space-charge model, we computed the energy modulation amplitude of an initial 120 MeV round uniform electron beam with 120 A current, 5% modulation, and zero initial temperature propagating through a drift space. Figure 1 shows the amplitude of energy modulation as a function of distance in comparison with an often used analytical model of longitudinal space-charge impedance [5]. This analytical model presupposes that the longitudinal component of the electric field across the beam is uniform and equal to the value on the beam axis. This is a good approximation if the wavelength of the perturbation as measured in the beam commoving frame is large compared to the beam transverse radius (or $k^* r_b/\gamma \ll 1$, where $k=2\pi/\lambda$ is the perturbation wavenumber in the lab frame.) However, as shown in the picture at smaller wavelengths the analytical model tends to overestimate the energy modulation when this is averaged over the beam tranasverse density. See also [6].

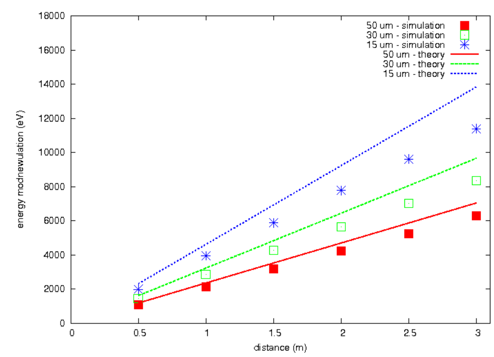

Figure 1: Energy modulation amplitude as a function of distance with initial 5% current modulation at 15 um, 30 um and 50 um wavelength.

The code is implemented on parallel computers using both a domain-decomposition method and a particle-field

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decomposition method. In the domain-decomposition method, the spatial physical domain is decomposed among processors. The particles located inside a physical domain are assigned to the processor containing that physical domain. The particle movement is controlled through a particle manager using neighboring communication. Dynamic load balance is used periodically to adjust the size of each domain. In the particle-field decomposition method, all particles and computational domain grids are uniformly distributed among all processors. Global communication is used to collect the particle charge density distribution on each physical domain. The Poisson equation is solved in parallel in both approaches. The particle-field decomposition method has the advantage of good load balance without resorting to any dynamic load balance. Its disadvantage is to use global communication to collect the charge density distribution.

The linac simulation starts with an initial distribution generated by the photoinjector. In most cases, this initial macroparticle distribution is generated by some other photoinjector simulation code such as ASTRA or IMPACT-T. The number of macroparticles in this initial distribution can be as small as a few hundred thousand or a few million. In order to suppress the sampling noise in that initial distribution, up-sampling is used with many more macroparticles, e.g. one billion macroparticles. In this study, a six-dimensional box centered at the original particle phase space location is used to up-sample the initial distribution. A uniform distribution is assumed in four-dimensional transverse phase space with box size set by external users. Within the box, a linear current density distribution is assumed using the current profile from the original particle distribution. The energy-position correlation is obtained from the original distribution using a cubic spline. Each new particle inside the box assumes the same uncorrelated energy spread as the original particle plus a Gaussian or uniformly sampled uncorrelated energy spread and a correlated energy from the new longitudinal position. The box size is chosen to produce sufficient smoothness of the resulting particle distribution while maintaining similar global properties (rms emittance, current profile, etc) of the original distribution. Figure 2 shows the initial peak current profile of a Gaussian distribution from direct one billion macroparticle sampling and from one billion macroparticle up-sampling of a two million Gaussian particle distribution. It is seen that the direct sampling and the up-sampling described above have a good agreement between each other. Figure 3 shows the final longitudinal phase space from the direct sampling and the up-sampling. Again, the up-sampling method used here gives a good reproduction of the direct sampling results.

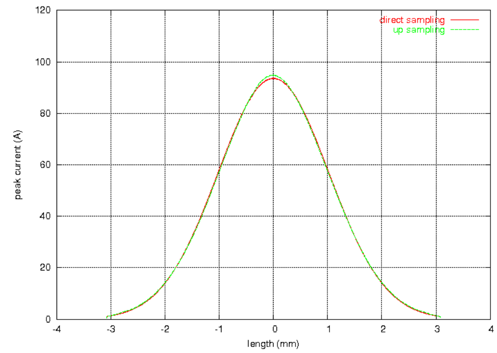

Figure 2: Initial current profile from direct sampling and up sampling.

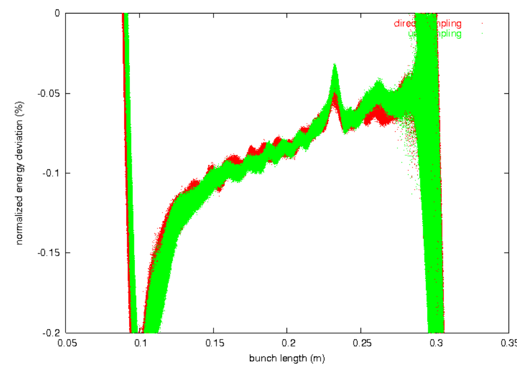

Figure 3: Final longitudinal phase space from direct sampling and up sampling.

NUMERICAL PARAMETER SETTINGS

The choice of numerical parameters in the self-consistent macroparticle simulation can significantly affect the final results due to the fact that the microbunching instability is highly sensitive to initial noise level. Figure 4 shows the final energy spread at the end of the linac as a function of number of macroparticles used in the simulation.

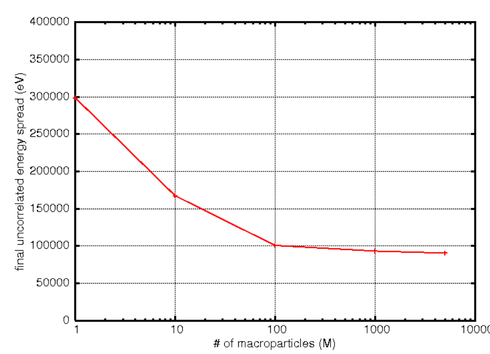

Figure 4: Final electron beam energy spread as a function of number of macroparticles.

It is seen that the final energy spread starts to saturate beyond 100 million macroparticles. Using a smaller number of macroparticles will lead to an unphysically larger energy spread. As the number of macroparticles approaches to the real number of electrons in the beam, the finite number of numerical grid points being used may present some unphysical smoothness of the electron beam. Figure 5 shows the power spectrum of the initial current profile from using 1024, 2048, 4096, and 8192 grid points. It is seen that the increasing number of grid points will mostly increase the initial current noise level at high frequency.

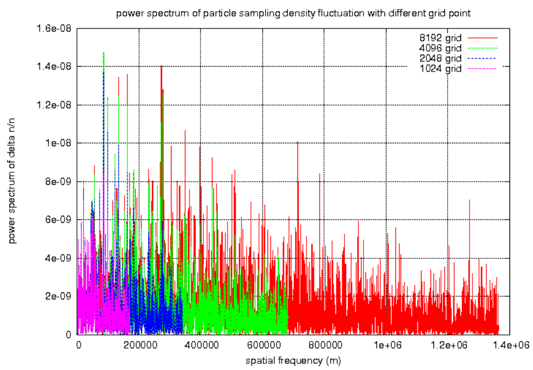

Figure 5: Power spectra of the initial current profile using different number of grid points.

Near the low frequency level, there is not much difference in the noise level for grid points beyond 2048. This suggests that keeping on increasing the number of grid points will not lead to an increase of noise level near low frequency. From the linear theory calculation, the gain of the microbunching instability decreases quickly at high frequency and has a peak near the low frequency in our linac study (around 300 um) [6]. This suggests that keeping on increasing the number of grid points will not change the final energy spread driven by the microbunching instability that is peaked near the low frequency level. Figure 6 shows the final energy spread with 2048 and 4096 grid points. It is seen that both cases give nearly the same final energy spread.

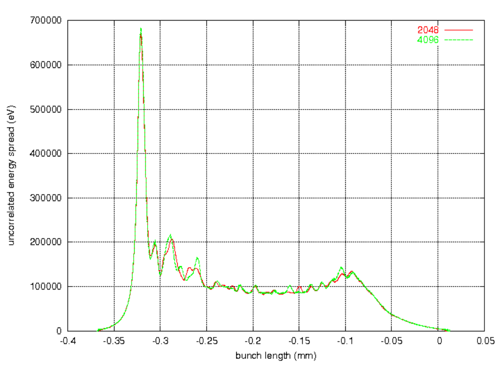

Figure 6: Final energy spread from simulations using 2048 and 4096 grid points.

APPLICATIONS

Using one billion macroparticles, we carried out self-consistent particle tracking of the electron transport subject to the microbunching instability in a linac planned for a soft X-ray free electron laser at Berkeley [7]. Given the same rms bunch length and similar peak current, the detailed shape of the initial current profile can have significant effects on final beam quality. Figure 7 shows the final energy spread for four different initial current distributions. Here, Litrack 1 and Litrack 2 are two initial distributions obtained from the back track of an ideal current profile at the end of the linac using the Litrack code.

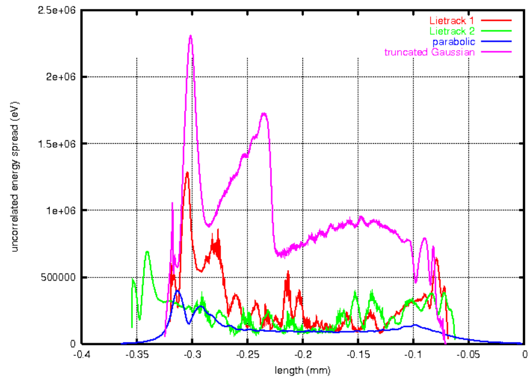

Figure 7: Final energy spread from using different initial current distributions.

It appears that the parabolic distribution with the same rms bunch length produces the best beam quality at the end of the linac. Using five billion macroparticles that is close to the real number of electrons in 0.8 nC charge, we simulated the electron beam transport through the linac for an array of soft X-ray FELs. The initial peak current is about 70 A with a parabolic density distribution and 5 keV uncorrelated rms energy spread. Figure 8 shows the longitudinal phase space distribution at the end of linac. The final rms energy spread is on the order of 0.01%. Figure 9 shows the horizontal and vertical slice emittance at the end of the linac. No slice emittance growth is seen from the simulation. Figure 10 shows the final current profile at 2.4 GeV energy. This current profile is reasonably flat enough for generating coherent soft X-ray radiation.

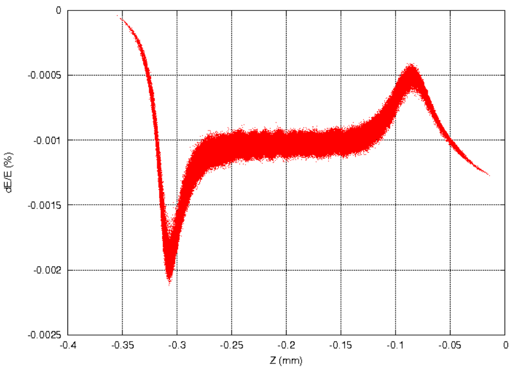

Figure 8: Longitudinal phase space distribution at the end of the linac from a five billion macroparticle simulation.

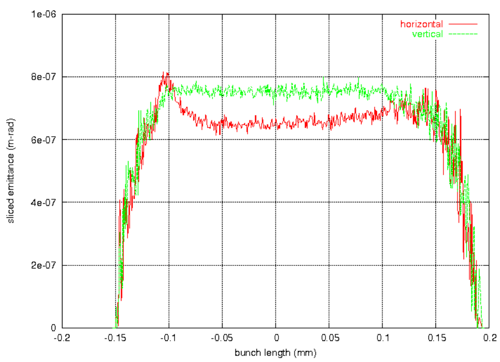

Figure 9: Transverse slice emittance at the end of the linac.

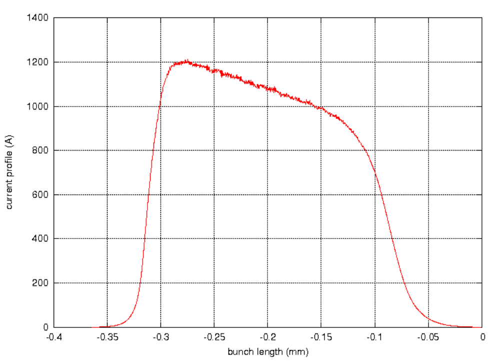

Figure 10: Current profile at the end of the linac.

The initial uncorrelated energy spread in an electron beam can smear the coherent growth of the microbunching instability. A larger initial energy spread leads to less growth of the microbunching instability. Figure 11 shows the final uncorrelated rms energy spread as a function of initial energy spread. It is seen that beyond 5 keV initial energy spread, the final energy shows a linear dependence of the initial energy spread due to the bunch compression. The microbunching instability has been sufficiently suppressed by the incoherent motion of electrons with different initial energy spread.

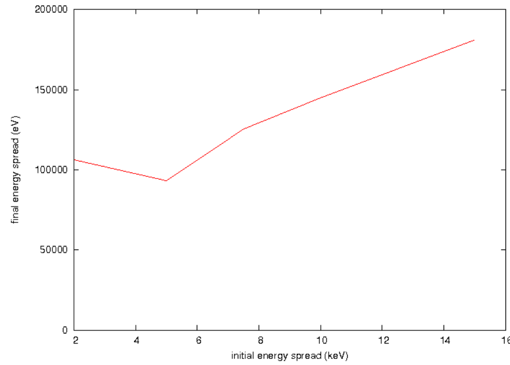

Figure 11: Final energy spread as a function of initial energy spread.

In conclusion, we have shown that a large number of macroparticles is needed for self-consistent particle tracking of high brightness electron beams subject to the microbunching instability in order to accurately predict the electron beam properties at the end of the linac. Applications of large-scale simulation with billions of macroparticles to the planned Berkeley FEL linac show that a reasonably good beam quality can be achieved to satisfy performance requirements for the soft x-ray FEL array.

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